הפקולטה להנדסה כימית

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GTEP Grand Technion Energy Program
תוכנית האנרגיה ע״ש גרנד

Wolfson Department of Chemical Engineering Seminar

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Theory of Water Purification by Electrochemical Systems

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Despite significant progress in electrochemical water purification, foundational theoretical gaps remain in accurately predicting system behavior under practical conditions—particularly regarding pH regulation, degradation pathways, and chemical kinetics. To address these challenges, we develop unifying theoretical and computational frameworks that span both desalination and reactive platforms, integrating mechanistic modeling, numerical simulation, and automated kinetic analysis.

One area of focus is electrodialysis (ED), for which we construct a spatially resolved model that captures pH dynamics at underlimiting current conditions. This model reveals the emergence of intra-stack acid–base gradients driven by water dissociation and coupled ion transport, offering quantitative insight into how bulk composition and applied voltage shape localized chemical environments in ED systems.

In parallel, we formulate a physics-based degradation model for capacitive deionization (CDI) that incorporates five coupled mechanisms: ion transport by electrodiffusion and advection, electroadsorption, Faradaic charge transfer, and pH-dependent surface reactions. This framework enables prediction of performance decline by tracking the spatial and temporal accumulation of reactive surface groups, providing mechanistic understanding of CDI aging under diverse operating conditions.

Complementing these efforts, we briefly introduce a computational chemistry workflow for the automated generation of pressure-dependent reaction mechanisms for formic acid decomposition. By benchmarking tools such as RMG, ARC, and T3, we evaluate predictive accuracy and identify systematic sources of error. While preliminary, this effort lays the groundwork for extending mechanism generation to purification–reactive electrochemical systems.

Together, these studies establish a theoretical foundation for electrochemical water treatment, advancing our ability to predict and control system behavior through detailed mechanistic insight and multi-scale simulation tools.